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Statistically Significant Trends in Triatomic Molecular Data Invite Theoretical Analysis

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Purpose

We analyzed data for several properties of main-group neutral triatomic molecules in order to identify global trends which would be useful in the construction of a triatomic molecular periodic system. This paper is concerned with the data for the 3 properties, namely S @ 298K, ΔH (formation), and IP, for which we have the most data and thus which provide the most accurate conclusions.

Methods

Our preliminary analysis was entirely graphical and involved both 2D and pseudo 4D plots of the molecular data. In preparing the 2D graphs we plotted the data verses various functions of the atoms' row and column numbers in order to find the function which resulted in a smooth curve. The best fit seems to be provided by the function R1*R2+R2*R3, as is shown by figure 1 which presents ionization potentials for molecules whose atoms come from row 2 on the periodic table.

The pseudo 4D graphs are cubes which use the 3 real axes for the atoms' column (group) numbers and represent the molecular properties either with colored dots or with different shapes which correspond to ranges for the data. Figure 2 shows a pseudo 4D graph of entropy for molecules from row 2.

With these graphs, we visually identified 2 global trends. The first consists of planes for which C1+C2+C3=constant. We called these planes isoelectronic sequences. They contain molecules with the same numbers of valence electrons. This trend is to be expected from elementary molecular orbital theory. The second trend consists of planes for which

(C1+C2)+(C2+C3)=constant. We call these bound-pair sequences.

After identifying the trends, we performed statistical analysis on the data to see if the variances (s_1^2) of the data along the trends was significantly lower than the aggregate variance (s_2^2) for all molecules from (R1,R2,R3). Next, we took each $s_1^2-s_2^2$ as a datum and used a t-test to determine to what extent the mean of these data differed from 0.

Results

The results of the statistical analysis were promising, though limited by the lack of data. In every case for molecules from (2,2,2), the isoelectronic sequences were t-test significant with $\alpha=.01$. Also for molecules from (2,2,2), the bound-pair sequence with C1+2C2+C3=18 was χ^2-test significant for entropy and dissociation potential. For data from all molecules, both normalized and unnormalized, the isoelectronic sequences were t-test significant, and the bound-pair sequences for entropy, dissociation potential, and log of the partition function were t-test significant.

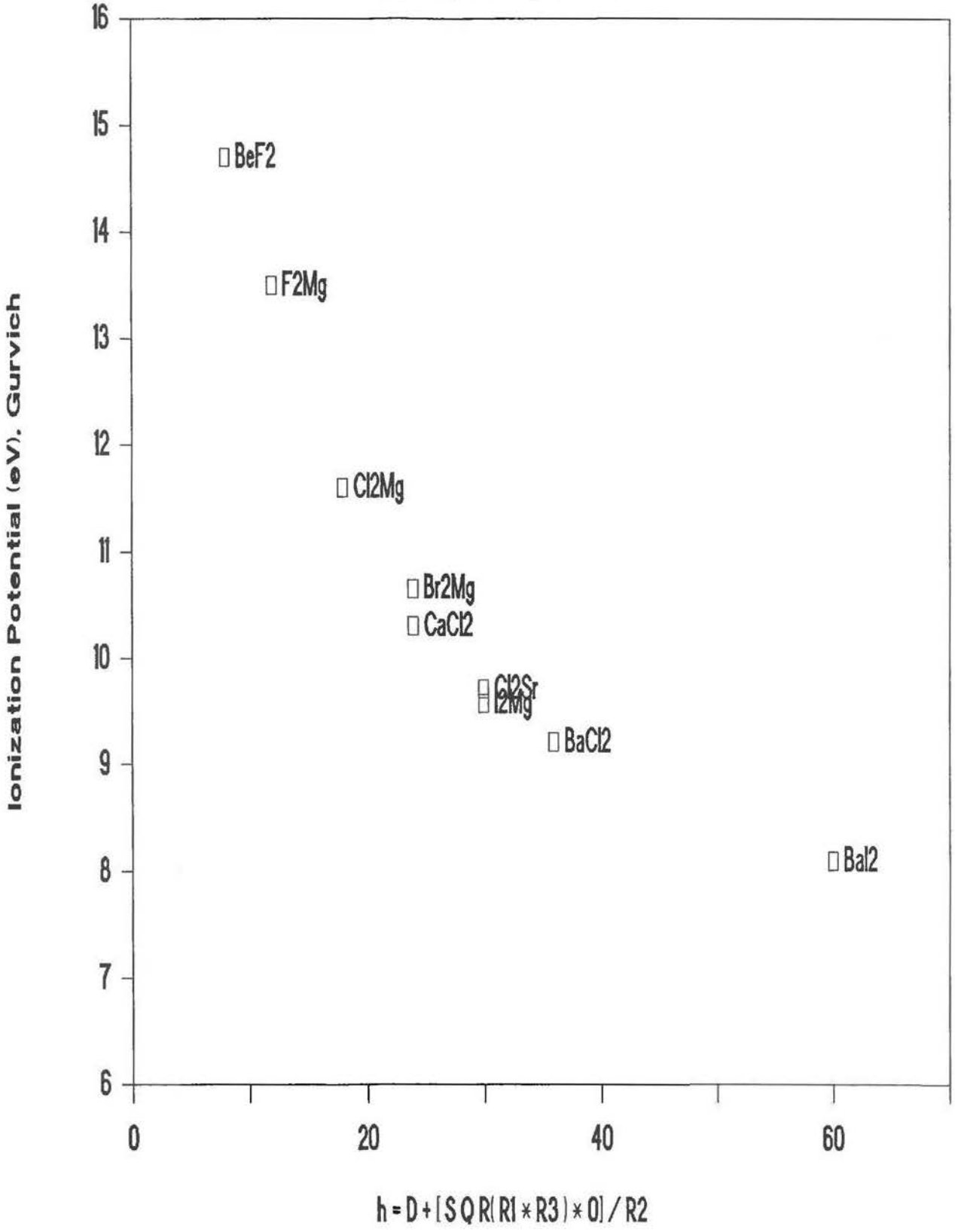
Conclusions

Our results suggest that quantum theorists should explore the usefulness, other than for ionization properties, of the relation $\Psi(1,2,3)=\Psi(1,2)+\Psi(2,3)$, where 1 and 3 are the outer atoms and 2 is the inner atom. Also, a more accurate analysis which includes error would be useful.

Figure 1

TRIATOMIC DATA

C1 = 31 C2 = 2 C3 = 31



S @ 298K (J/K-Mole), from JANAF82